

```

// masscap.cpp : Defines the entry point for the console application.
//

/* Ken Black 4/28/99

This program reads a time series of concentrations at each nodal point
of extraction and
injection wells. This information is generated with the postproc
program written by Steve Andreson.
This program computes mass capture statistics from the concentration
information.
This program is applicable for all box models.

```

```

argv[1] = post proc output file
argv[2] = modified well file - time must be added to the number of nodes
header for each stress period
argv[3] = output file name

```

Updated on 9/30/04 to be in sync with post-proc output.

The number of lines being read in the well_hist.sum file has been changed from 10 to 13.
 You still need to add the initial mass tag at the beginning, and this comes from the concentration.sum file from post proc.

Here is the batch file to run this program:

```
m:\data\c\source\masscap\debug\masscap wellhist.sum c2003.wtm c2003mc.out
```

The contents of wellhist.sum

```

im 494.13 <- This has to be manually added to this file
con="c2003.CON 9/29/2004 10:49:04 PM 482014400 bytes"
btn="c2003.btn 1/11/2000 8:36:10 PM 36677596 bytes"
bas="c2003.bas 9/29/2004 8:19:40 PM 29420590 bytes"
bcf="c2003.bcf 9/29/2001 8:24:24 PM 28906226 bytes"
no mask file
sit="c2003.sit 9/30/2004 2:57:28 PM 3898 bytes"
easting=1959840
northing=298040
rotation=0.0
NMonitor=421
NTime=51.0
      Well ID      Easting      Northing      Elevation      Col      Row      Lay
      Time          Value (head or conc)
      AM20        1976501.7      305564.9       -185.0        81      206      27
      0.0000      0.00000
      356.2500     0.00000

```

The contents of c2003.wtm

```
421          0 <- starting time, this has only one stress period
```

```

1      185      30  -1657.36      0.00 AM06
2      185      30  -8233.36      0.00 AM06
3      185      30  -8179.89      0.00 AM06
4      185      30  -8233.35      0.00 AM06
.....
*/



#include <stdio.h>
#include <stddef.h>
#include <stdlib.h>
#include <stdarg.h>
#include <string.h>
#include <malloc.h>
#include <dos.h>
#include <float.h>
#include <math.h>

/******Preprocessor Directives
*****/


#define mass_convert    28.3/1000000 /* convert ug/l*ft^3/day to g/day
*/
#define max_time_steps 160 /* maximum number of time steps */
#define max_nodes      10000 /* maximum number of observation (nodal)
points - this is not equal to the
                                number of wells since each well usually
has more than one nodal point */
#define max_well       500 /* maximum number of unique wells */
#define blank_lines    13 /* the number of lines to read at the
beginning of the well_hist.sum */
#define true 1
#define false 0

/****** Data Structure Definitions
*****/


struct concentration { /* these are the nodal concentrations, flow
rates, etc over time */
    char wellid[20];           /* MMR well id */
    float easting;             /* ft MA state plane */
    float northing;            /* ft MA state plane */
    float elevation;            /* ft msl */
    float time[max_time_steps]; /* days */
    float conc[max_time_steps]; /* parts per billion */
    float flow_rate[max_time_steps]; /* flow in ft^3/day */
    float nodal_mass_flux[max_time_steps]; /* flow in ft^3/day */
    float nodal_mass_removed[max_time_steps]; /* total mass removed at
the node at end of simulation */
    float total_water_pumped[max_time_steps]; /* total flow removed
from the node */
}

```

```

        int row;                      /* row number          */
        int col;                      /* column number       */
        int lay;                      /* layer number        */
    };
struct concentration wellconc[max_nodes];

struct wellflow { /* these are the nodal flows which can be time varying
(read from modified *.wel file) */
    int   row[max_nodes];         /* row number          */
    int   col[max_nodes];         /* column number       */
    int   lay[max_nodes];         /* layer number        */
    int   numwell;               /* num wells per ts   */
    float time;                  /* days                */
    float flow_rate[max_nodes];  /* flow ft3/day        */
};
struct wellflow nodeflow[max_time_steps];

struct welltotal { /* these are the totals for each well */
    int nodes_per_well; /* number of nodes per well */
    float total_mass;   /* well accumulative mass recovery */
    float total_pump;  /* total volume pumped from the well */
    float gal_gram;    /* total gallons removed per gram recovered */
    float inf_conc;   /* average influent concentration */
    float total_flow; /* total flow in ft^3/day for the well */
    float nod_conc;   /* conc*flow at each node */
};
struct welltotal wellsum[max_well];

/********************* Global Variables
***** */

FILE *summary_file;
char input_file1[120],input_file2[120],input_file3[120];
int num_stress_periods,total_nodes,total_time_steps,unique_wells,tpt; /*
tpt = time pointer */
float initial_mass;

/********************* function declarations
***** */

void Abort(char*mess);
void Abort_nodes(int);
void Abort_times(int);
void Abort_ini_mass(void);
void Abort_well(int);
void accumulate_well_data(void);
void link_flow_conc(void);
int main(int,char **);
void process_nodal_concentration_data(void);
void read_concentration_data(void);
void read_flow_data(void);

```

```

***** Main *****
***** */

int main(int argc,char*argv[]){
    strcpy(input_file1,argv[1]); /* post proc output file */
    strcpy(input_file2,argv[2]); /* modified well file - time added to
each stress period */
    strcpy(input_file3,argv[3]); /* output file name */
    read_concentration_data();
    read_flow_data();
    link_flow_conc();

    process_nodal_concentration_data();
    accumulate_well_data();
    return(1);

}

***** Abort *****
***** */

void Abort(char*mess)                                /* write message and exit */
{
    fprintf(stderr,"\nfile open error: %s\n",mess);
    fprintf(summary_file,"\\nfile open error: %s\\n",mess);
    fcloseall();
    exit(1);
}

***** Abort_well *****
***** */

void Abort_well(int numwell)                         /* write message and
exit */
{
    fprintf(summary_file,"\\nMaximum number of wells is: %d\\n",max_well);
    fprintf(summary_file,"\\nCurrent number of wells is: %d\\n",numwell);
    fprintf(stderr,"\\nMaximum number of wells is: %d\\n",max_well);
    fprintf(stderr,"\\nCurrent number of wells is: %d\\n",numwell);
    fcloseall();
    exit(1);
}

***** Abort_nodes *****
***** */

void Abort_nodes(int numnodes)                      /* write message and
exit */
{
    fprintf(summary_file,"\\nMaximum number of nodes is: %d\\n",max_nodes);
    fprintf(summary_file,"\\nCurrent number of nodes is: %d\\n",numnodes);
    fprintf(stderr,"\\nMaximum number of nodes is: %d\\n",max_nodes);
    fprintf(stderr,"\\nCurrent number of nodes is: %d\\n",numnodes);
    fcloseall();
    exit(1);
}

```

```

}
***** Abort_times ****
***** Abort_times ****

void Abort_times(int numtimes) /* write message and exit */
{
    fprintf(summary_file, "\nMaximum number of timesteps is:
%d\n", max_time_steps);
    fprintf(summary_file, "\nCurrent number of timesteps is:
%d\n", numtimes);
    fprintf(stderr, "\nMaximum number of timesteps is:
%d\n", max_time_steps);
    fprintf(stderr, "\nCurrent number of timesteps is: %d\n", numtimes);
    fcloseall();
    exit(1);
}

*****
***** Abort_times ****
***** Abort_times **/


void Abort_ini_mass(void) /* write message and exit */
{
    fprintf(summary_file, "\nInitial mass has not been added to first line
of: %s\n", input_file1);
    fprintf(stderr, "\nInitial mass has not been added to first line of:
%s\n", input_file1);
    fcloseall();
    exit(1);
}

*****
***** accumulate_well_data ****
***** accumulate_well_data **/


void accumulate_well_data(void) {
int j,k,n,local_node_counter,global_node_number,gnpt;

/* calculate nodal mass flux for each well for each time step */
fprintf(summary_file, "n*****\n*****\n");
fprintf(summary_file, "Table 4. Summary of contaminant recovery for each
well over time\n\n");
fprintf(summary_file, "Accumulative Mass Removed - mass_rem (kg) \n");
fprintf(summary_file, "Percent Initial Mass = perc init mass - this is
calculated based on dissolved mass+adsorbed mass\n");
fprintf(summary_file, "Total Water Pumped from Well = h20_pump (millions
of gallons)\n");
fprintf(summary_file, "Total Flow Rate = tot_flow (gal/min) from each
extraction/injection well\n");
fprintf(summary_file, "Gallons Pumped Per Gram Recovered = gallon per gram
(gal/gm)\n");
fprintf(summary_file, "Computed Influent Concentration = inf_conc
(ppb)\n");
fprintf(summary_file, "Initial Mass Read From File = %10.2f
(kg)\n\n", initial_mass);
}

```

```

fprintf(summary_file,"well      easting      northing      time      mass_rem
perc_init    h20_pump      tot_flow      gallon      inf_conc\n");
fprintf(summary_file,"id          (ft)        (ft)        (yr)        (kg)
mass         (mil_gal)    (gpm)       per_gram     (ppb)\n");

global_node_number=0; /* this moves the array pointer from 0 to number
of observation nodes */

for(k=0;k<unique_wells;k++) {
    wellsum[k].total_mass=0;
    wellsum[k].total_pump=0;
    wellsum[k].gal_gram=0;
    wellsum[k].inf_conc=0;

    for(j=0;j<total_time_steps;j++) {
        local_node_counter=0;
        for(n=0;n<wellsum[k].nodes_per_well;n++) {
            gnpt=global_node_number+local_node_counter; /* global
node pointer */
            if(j==0){
                /* initialize totals */

wellsum[k].total_mass+=(wellconc[gnpt].nodal_mass_removed[j]);
wellsum[k].total_pump+=(wellconc[gnpt].total_water_pumped[j]);
wellsum[k].total_flow+=(wellconc[gnpt].flow_rate[j]);

wellsum[k].nod_conc+=(wellconc[gnpt].conc[j]*wellconc[gnpt].flow_rate[j])
;
            }
            else {
                /* since nodal mass removed is stored as an
accumulative total, I must subtract the previous value */

wellsum[k].total_mass+=(wellconc[gnpt].nodal_mass_removed[j]-
wellconc[gnpt].nodal_mass_removed[j-1]);

wellsum[k].total_pump+=(wellconc[gnpt].total_water_pumped[j]-
wellconc[gnpt].total_water_pumped[j-1]);
wellsum[k].total_flow+=(wellconc[gnpt].flow_rate[j]-
wellconc[gnpt].flow_rate[j-1]);
wellsum[k].nod_conc+=(wellconc[gnpt].conc[j]*
wellconc[gnpt].flow_rate[j])-
(wellconc[gnpt].conc[j-
1]*wellconc[gnpt].flow_rate[j-1]);}

            local_node_counter++;
        }

wellsum[k].gal_gram=wellsum[k].total_pump/wellsum[k].total_mass;
if(wellsum[k].gal_gram>150000||wellsum[k].total_pump<10) /* this
is an injection well - set value to 0, or beginning of pumping */
wellsum[k].gal_gram=0;

```

```

/* compute average influent concentration only if well is
pumping*/
    if(wellsum[k].total_flow>(float)0.)

wellsum[k].inf_conc=wellsum[k].nod_conc/wellsum[k].total_flow;
else
    wellsum[k].inf_conc=0.0;
if(wellsum[k].inf_conc<0.00001) /* less than detection */
    wellsum[k].inf_conc=0;

        fprintf(summary_file,"%s %10.2f %10.2f %10.2f %10.4f %10.2f
%10.1f %10.2f %10.1f %10.5f\n",
wellconc[global_node_number].wellid,
wellconc[global_node_number].easting,
wellconc[global_node_number].northing,
wellconc[global_node_number].time[j],
wellsum[k].total_mass/1000, /* convert to kg */
wellsum[k].total_mass/1000/initial_mass*100, /* convert to
kg, divide by initial mass, convert to percent */
wellsum[k].total_pump/1000000, /* convert to million gallons
*/
wellsum[k].total_flow/1440*7.48, /* flow rate in
gallons/minute */
wellsum[k].gal_gram, /* gallons pumped per gram
contaminant recovered */
wellsum[k].inf_conc); /* average influent
concentration */

}

global_node_number+=local_node_counter;

/* fprintf(summary_file,"\n"); */

}

***** process_nodal_concentration_data
***** */

void process_nodal_concentration_data(void){
int j,k;

/* calculate nodal mass flux for each well for each time step */
fprintf(summary_file,"*****\n*****\n");
fprintf(summary_file,"Table 3. Summary of nodal concentration data and
accumulative mass removal over time \n\n");
fprintf(summary_file,"well      easting      northing      elevation      time
concen      flow_rate      nod_mflux      mass_rem      h2o_pump\n");
fprintf(summary_file,"id          (ft)          (ft)          (ft)          (yr)
(uq/l)      (ft^3/d)      (q/day)      (q)      (thousand gal)\n");

```

```

for(k=0;k<total_nodes;k++) {

    for(j=0;j<total_time_steps;j++) {
        wellconc[k].nodal_mass_removed[j]=0;
        wellconc[k].total_water_pumped[j]=0;

wellconc[k].nodal_mass_flux[j]=(float)fabs((double)(wellconc[k].conc[j]*wellconc[k].flow_rate[j]*(float)mass_convert));

        if(j>=1){ /* sum up mass removed at each node and total water pumped */
            wellconc[k].nodal_mass_removed[j]=(wellconc[k].nodal_mass_flux[j-1]+wellconc[k].nodal_mass_flux[j])/(float)2.
                                         *(wellconc[k].time[j]-
wellconc[k].time[j-1])*(float)365.25+
wellconc[k].nodal_mass_removed[j-1];

wellconc[k].total_water_pumped[j]=(float)(fabs((double)(wellconc[k].flow_rate[j-1]+wellconc[k].flow_rate[j]))/(float)2.
                                         *(wellconc[k].time[j]-
wellconc[k].time[j-1])*(float)365.25*(float)7.48+
wellconc[k].total_water_pumped[j-1]);}

        fprintf(summary_file,"%s %10.2f %10.2f %10.2f %10.2f %10.2f %10.2f
%10.2f %10.2f %10.0f\n",
wellconc[k].wellid,
wellconc[k].easting,
wellconc[k].northing,
wellconc[k].elevation,
wellconc[k].time[j],
wellconc[k].conc[j],
wellconc[k].flow_rate[j],
fabs((double)wellconc[k].nodal_mass_flux[j]),
wellconc[k].nodal_mass_removed[j],
wellconc[k].total_water_pumped[j]/1000 /* convert to thousand gallons */);
    }

/* fprintf(summary_file,"\n"); */

}

```

```

***** link_flow conc *****/

```

```

/* this routine finds the flow rate that is applicable for every
concentration time step stored in the file */

void link_flow_conc(void ){
int j,k,n,tm,tpt,wellfound,nspl; /* tpt = time pointer */
float cur_time;

nspl=num_stress_periods+1;

for(k=0;k<total_nodes;k++){ /* process every observation node */

    for(n=0;n<total_time_steps;n++){ /* for each time step, find
the appropriate flow */
        cur_time=wellconc[k].time[n]; /* initialize time */

        for(tm=0;tm<nspl;tm++){ /* time look-up: check if same
time or less than next time */
            if(fabs((double)(cur_time-
(nodeflow[tm].time/(float)365.25)))<0.01){ /* exact time match */

                tpt=tm;
                /* fprintf(summary_file,"Exact Time Match: cur
time = %6.2f node time =%6.2f and timeptr = %d
\n",cur_time,(nodeflow[tpt].time/365.25),tpt); */
                else
if((cur_time>(nodeflow[tm].time/(float)365.25))&&(cur_time<(nodeflow[tm+1]
.time/(float)365.25))){ /* in between time intervals */
                tpt=tm;
                /* fprintf(summary_file,"cur time = %6.2f node
time1 =%6.2f node time2 =%6.2f and timeptr = %d
\n",cur_time,(nodeflow[tm].time/365.25),(nodeflow[tm+1].time/365.25),tm);
*/
            }
        }

    } /* end time step loop */

    for(j=0;j<nodeflow[tpt].numwell;j++){ /* process from 0 to
number of wells to match i,j,k at that time step */
        wellfound=false;

        if((nodeflow[tpt].row[j]==wellconc[k].row)&&(nodeflow[tpt].col[j]==
wellconc[k].col)&&(nodeflow[tpt].lay[j]==wellconc[k].lay)){ /* match
found */
            wellconc[k].flow_rate[n]=nodeflow[tpt].flow_rate[j];
            fprintf(summary_file,"flow rate = %10.2f for well %19s
at time %6.2f yr at row=%3d col=%3d
layer=%2d\n",nodeflow[tpt].flow_rate[j],wellconc[k].wellid,cur_time,wellc
onc[k].row,wellconc[k].col,wellconc[k].lay);
            wellfound=true;
            break;
        }

    } /* end j loop */
    if(!wellfound){ /* no entry found for well at this time
- set value to 0 */
        wellconc[k].flow_rate[n]=0.;


```

```

                fprintf(summary_file,"Warning: no entry found for
well %19s at time %6.2f yr so rate is being set to:
\n",wellconc[k].wellid,cur_time);
                fprintf(summary_file,"flow rate = %10.2f for well
%19s at time %6.2f yr at row=%3d col=%3d
layer=%2d\n",wellconc[k].flow_rate[n],wellconc[k].wellid,cur_time,wellcon
c[k].row,wellconc[k].col,wellconc[k].lay); }

        } /* end stress period loop */
    } /* end k loop */
} /* end function */

/********************* read_concentration_data
***** */

void read_concentration_data(void){

FILE *file;
char bufr[120],dummystr[25];
int i,n,k,npw;
float maxelev,minelev;

/* open input data summary file */

if((summary_file=fopen(input_file3,"wt"))==NULL){
    printf("can't open the transport data summary ouput file");
    Abort(input_file3);}
else
    printf("\nData summary output file %s is open!\n",input_file3);

/* open concentration file - need to use input_file for filename after
debugging */

if((file=fopen(input_file1,"rt"))==NULL){
    printf("can't open the nodal concentration file");
    Abort(input_file1);}
else
    printf("\nConcentration file %s from post-proc is
open!\n",input_file1);

fprintf(summary_file,"\nThis transport output file is :
%s",input_file3);
fprintf(summary_file,"\nThe concentration data file is:
%s",input_file1);
fprintf(summary_file,"\nThe nodal flow data file is    :
%s\n",input_file2);

fprintf(summary_file,"***** CURRENT PROGRAM LIMITS
*****\n");
fprintf(summary_file,"Maximum Number of Wells      :
%d\n",max_well);
}

```



```

        minelev=(minelev<wellconc[n-1].elevation) ? minelev :
wellconc[n-1].elevation;
                wellsum[unique_wells].nodes_per_well=npw;
                fprintf(summary_file,"Well %19s contained %3d nodes
between %10.2f ft and %10.2f ft\n",wellconc[n-
1].wellid,wellsum[unique_wells].nodes_per_well,maxelelev,minelev);
                minelev=100000;
                maxelelev=-100000;
                npw=1;
                unique_wells++;
                if(unique_wells>max_well)
                        Abort_well(unique_wells);
        }
    }
    n++;
    if(n>max_nodes)
        Abort_nodes(n);

    k=0;
}
else /* n must be decremented back one! */
if(sscanf(bufr,"%f%f",&wellconc[n-1].time[k],&wellconc[n-
1].conc[k]==2){
        /* convert time to years */
        wellconc[n-1].time[k]/=365.25;
/*        printf("%10.2f %10.2f\n",wellconc[n-1].time[k],wellconc[n-
1].conc[k]); */

        k++;
        if(k>max_time_steps)
            Abort_times(k);
    }

/*
 * process last record */
maxelelev=(maxelelev>wellconc[n-1].elevation) ? maxelelev : wellconc[n-
1].elevation;
minelev=(minelev<wellconc[n-1].elevation) ? minelev : wellconc[n-
1].elevation;
wellsum[unique_wells].nodes_per_well=npw;
fprintf(summary_file,"Well %19s contained %3d nodes between %10.2f
ft and %10.2f ft\n",wellconc[n-
1].wellid,wellsum[unique_wells].nodes_per_well,maxelelev,minelev);

total_nodes=n;
total_time_steps=k;
unique_wells++;

/* write summary data */

fprintf(summary_file,"\n\nTotal well nodes = %d\n",total_nodes);
fprintf(summary_file,"Total wells (unique well ids)  =
%d\n",unique_wells);

```

```

        fprintf(summary_file,"Total concentration time steps =
%d\n\n",total_time_steps);

fclose(file);

}

***** read_flow_data *****/
void read_flow_data(void){

FILE *file2;
char bufr[120];
int n,timecount;
float time_yr;

/* open nodal based well file */

if((file2=fopen(input_file2,"rt"))==NULL){
    printf("Can't open the modified modflow well/time file");
    Abort(input_file2);}
else
    printf("\nModified flow rate file %s is open!\n",input_file2);

fprintf(summary_file,"\n*****\n*****\n");
fprintf(summary_file,"Table 2. Summary of flow rates on a nodal basis
obtained from file: %s \n\n",input_file2);

timecount=0;

while(fgets(bufr,sizeof(bufr),file2)) {

if(sscanf(bufr,"%d%f",&nodeflow[timecount].numwell,&nodeflow[timecount].t
ime)==2){ /* go read layer,row,col,flow */
    time_yr=nodeflow[timecount].time/(float)365.25;
    fprintf(summary_file,"Well stress period #3d = %10.2f
years has %3d nodes \n",timecount+1,time_yr,nodeflow[timecount].numwell);
    /* handle situation where -1 can be used in the well
file to indicate the use of previous time step */
    if(nodeflow[timecount].numwell==-1){ /* use previous values
*/
        for(n=0;n<nodeflow[timecount-1].numwell;n++){
            nodeflow[timecount].numwell=nodeflow[timecount-
1].numwell;
            nodeflow[timecount].lay[n]=nodeflow[timecount-
1].lay[n];
            nodeflow[timecount].row[n]=nodeflow[timecount-
1].row[n];
            nodeflow[timecount].col[n]=nodeflow[timecount-
1].col[n];
}
}
}
}
}

```

```

        nodeflow[timecount].flow_rate[n]=nodeflow[timecount-
1].flow_rate[n];}
    }else
        for(n=0;n<nodeflow[timecount].numwell;n++) {
            fgets(bufr,sizeof(bufr),file2);

            sscanf(bufr,"%d%d%d%f",&nodeflow[timecount].lay[n],&nodeflow[timeco-
unt].row[n],&nodeflow[timecount].col[n],&nodeflow[timecount].flow_rate[n]
);
            /* convert negative flows to positve values */
            if(nodeflow[timecount].flow_rate[n]<(float)0.0)
                nodeflow[timecount].flow_rate[n]*=(float)-1.0;
/* debug statement      fprintf(summary_file,"stress period # %d %d %d
%f
\n",timecount+1,nodeflow[timecount].lay[n],nodeflow[timecount].row[n],nod-
eflow[timecount].col[n],nodeflow[timecount].flow_rate[n]); */
        }
        timecount++;
    }
    num_stress_periods=timecount;

}

/* set very large time for next array space */
nodeflow[timecount].time=(float)3652500.;
fprintf(summary_file,"Well stress period # %3d = %10.2f years has been
set for interpolation
usage\n",timecount+1,nodeflow[timecount].time/365.25);
    fprintf(summary_file,"Total number of actual stress periods = %d
\n\n\n",num_stress_periods);

fclose(file2);
}

```